Abstract for an Invited Paper
for the MAR09 Meeting of
The American Physical Society

Tuning the ionization energy of organic semiconductor films: The role of intramolecular polar bonds

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While an isolated individual molecule has only one ionization energy (IE), multiple values are found for molecules in ordered assemblies. Photoelectron spectroscopy of archetypical conjugated organic compounds combined with first-principles calculations and electrostatic modeling reveal the existence of a surface dipole built into molecular layers. Its origin lies in intramolecular polar bonds (IPBs) of the individual molecules, and its magnitude depends on the orientation of molecules relative to the surface of an ordered assembly. Suitable pre-patterning of substrates to induce specific molecular orientations in subsequently grown films thus permits adjusting the IE of one molecular species over up to 1 eV via control over layer morphology. Furthermore, mixing of differently terminated molecules (different IPBs) on a molecular length scale allows continuously tuning the IE of thin organic films between the limiting values of the two pure materials. Surface engineering of organic semiconductors via adjusting the polarity of intra-molecular bonds represents thus a viable alternative for controlling the energetics at organic/(in)organic interfaces.